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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/053,354	11/02/2001	Dan E. Rosenthal	020910-000210US	5806
28393	7590	07/19/2005	EXAMINER	
STERNE, KESSLER, GOLDSTEIN & FOX P.L.L.C. 1100 NEW YORK AVE., N.W. WASHINGTON, DC 20005			LUU, CUONG V	
			ART UNIT	PAPER NUMBER
			2128	

DATE MAILED: 07/19/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary	Application No.	Applicant(s)	
	10/053,354	ROSENTHAL, DAN E.	
	Examiner	Art Unit	
	Cuong V. Luu	2128	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
 - If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
 - If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
 - Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).
- Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) Responsive to communication(s) filed on 02 November 2001.
- 2a) This action is FINAL. 2b) This action is non-final.
- 3) Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) Claim(s) 1-33 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) Claim(s) _____ is/are allowed.
- 6) Claim(s) 1-33 is/are rejected.
- 7) Claim(s) _____ is/are objected to.
- 8) Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) The specification is objected to by the Examiner.
- 10) The drawing(s) filed on _____ is/are: a) accepted or b) objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) All b) Some * c) None of:
1. Certified copies of the priority documents have been received.
 2. Certified copies of the priority documents have been received in Application No. _____.
 3. Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- 1) Notice of References Cited (PTO-892)
- 2) Notice of Draftsperson's Patent Drawing Review (PTO-948)
- 3) Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08)
Paper No(s)/Mail Date _____ **5 PAGES**
- 4) Interview Summary (PTO-413)
Paper No(s)/Mail Date _____
- 5) Notice of Informal Patent Application (PTO-152)
- 6) Other: _____

Specification

1. The disclosure is objected to because of the following informalities:
 - 1.1. The inventors cited "Fig. 4". This figure does not exist.
 - 1.2. The disclosure is missing application numbers for cited U.S. Applications (page 4, line 26; p. 7, line 5; p. 8, line 25; p. 21, line 2).

Appropriate correction is required.

Claim Objections

2. Claims 6 and 25 are objected to because of the following informalities:
 - 2.1.1. As per claim 6, it recites the limitation "wherein q corresponds to internal coordinates" in line 1. The term "q" is not mentioned in claims that claim 6 depend on.
 - 2.1.2. As per claim 25, it recites the limitation "wherein q corresponds to internal coordinates" in line 1. The term "q" is not mentioned in claims that claim 6 depend on.

Appropriate correction is required.

Claim Rejections - 35 USC § 102

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

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(a) the invention was known or used by others in this country, or patented or described in a printed publication in this or a foreign country, before the invention thereof by the applicant for a patent.

Claims 1-2, 12-21, and 31-33 are rejected under 35 U.S.C. 102(a) as being unpatentable by the applicant's admitted prior art.

3. As per claim 1, the applicant's admitted prior art teaches a method of computer modeling the behavior of a molecule or set of molecules, comprising
 - selecting a model for said molecules, said model having equations of motion for said molecule (p. 3, lines 11-19; p. 6, lines 11-15);
 - formulating said equations of motion in Residual Form (p. 3, lines 32-34; p. 4, lines 1-3); and
 - integrating said model equations with an implicit integrator; whereby computer calculations for said molecular behavior are reduced (4, lines 10-12).

4. As per claim 2, the applicant's admitted prior art teaches said equations of motion in Residual Form comprise

$$\rho_q = q' - W(q).u$$

$$\rho_u = M(q).u' - f(t,q,u)$$

(u' and q' here are equivalent to u and q with a dot right above, respectively, due to issue with not being able to insert u or q with a dot right above the alphabets, respectively).

where q represents generalized system coordinates, u represents generalized velocities, W represents a generalized joint map matrix, M represents generalized system mass, f represents generalized system forces, and t represents time (p. 6, lines 11-32; p. 7, lines 1-13. The 2 equations presented in matrix format are not new.

Only terms q' and u' are derived differently using the well-known technique, implicit Euler integration, and then substituted to the direct-form equations, admitted as prior art by the applicant).

5. As per claim 12, the applicant's admitted prior art teaches said implicit integrator comprises an L-stable integrator (p. 7, lines 1-3).
6. As per claim 13, the applicant's admitted prior art teaches said L-stable integrator comprises an integrator from the group comprising implicit Euler, Radau5, SDIRK3, SDIRK4 and other implicit Runge-Kutta methods.
7. As per claim 14, the applicant's admitted prior art teaches said implicit integrator comprises an integrator from the group comprising DASSL and other implicit multi-step methods for ODE or DAE systems (p. 4, lines 3-6).
8. As per claim 15, the applicant's admitted prior art teaches a method of computer modeling the behavior of a molecule, said molecule having a plurality of bodies having masses, said method comprising
 - selecting a model for said molecule, said model having equations of motion for said molecule (p. 3, lines 11-19; p. 6, lines 11-15);
 - integrating said model equations with an implicit integrator; whereby computer calculations for said molecular behavior are reduced (4, lines 10-12).
 - formulating said equations of motion such that mass matrices corresponding to said masses for said plurality of bodies are not inverted (p.6, lines 20-24);

9. As per claim 16, this limitation has already been discussed in claim 1. It is, therefore, rejected for the same reasons.

10. As per claim 17, these limitations have already been discussed in claim 12. They are, therefore, rejected for the same reasons.

11. As per claim 18, these limitations have already been discussed in claim 13. They are, therefore, rejected for the same reasons.

12. As per claim 19, this limitation has already been discussed in claim 14. It is, therefore, rejected for the same reasons.

13. As per claim 20, computer code for modeling the behavior of a molecule, said code comprising

a model for said molecule, said model having equations of motion for said molecule, said equations of motion formulated in Residual Form (p. 4, lines 1-3; p. 3, lines 11-19; p. 6, lines 11-15); and

The applicant's admitted prior art teaches an implicit integrator for integrating said model equations over time (p. 4, 1-4; p. 2, lines 19-24).

As per claim 21, these limitations have already been discussed in claim 2. They are, therefore, rejected for the same reasons.

14. As per claim 31, these limitations have already been discussed in claim 12. They are, therefore, rejected for the same reasons.

15. As per claim 32, these limitations have already been discussed in claim 13. They are, therefore, rejected for the same reasons.

16. As per claim 33, this limitation has already been discussed in claim 14. It is, therefore, rejected for the same reasons.

Claim Rejections - 35 USC § 103

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

Claims 3-10, and 22-29 are rejected under 35 U.S.C. 103(a) as being unpatentable over applicant's admitted prior art as applied to claim 1, 2, and 20 above, and further in view of Michael Hollars et al (SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamic Inc.).

17. As per claim 3, the applicant's admitted prior art does not teach said integrating step is performed iteratively and residuals ρ_q and ρ_u are reduced below predetermined amounts before a next iterative integration step is performed.

However, Hollars et al teach these features (p. T-15, paragraph 5, lines 1-5. The examiner interprets time-step integrator as integration is performed iteratively.)

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art and Hollars. Hollars's teachings of integrating step performed iteratively and residuals ρ_q and ρ_u reduced below predetermined amounts before a next iterative integration step is performed would have helped incorporate the Residual Form equations successfully in order to converge to solutions faster which would in turn reduce time and resource to solve the equations.

18. As per claim 4, the applicant's admitted prior art does not teach model comprises a plurality of rigid bodies, each rigid body representing a portion of said molecule, and a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies.

However, Hollars et al teach these features (p. T-10, paragraph 4, lines 1, 2, 3; paragraph 7, lines 1-6)

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art and Hollars et al since molecular structures are very similar to those structures described in Hollars' manual. Hollars et al's teaching of model comprises a plurality of rigid bodies, each rigid body representing a portion of said molecule, and a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies would have helped model molecules to apply Residual Form equations effectively.

19. As per claim 5, Hollars et al teach each hinge connection comprise a connection selected from the group comprises a slider joint, a pin joint, a ball joint, a free

connection, and combinations thereof (p. T-10, paragraph 7, lines 1-6; p.T-11, paragraph 1).

20. As per claim 6, the applicant's admitted prior art teaches q corresponds to internal coordinates of one of said rigid bodies with respect to another of said rigid bodies (p. 6, lines 15-16).

21. As per claim 7, the applicant's admitted prior art teaches said internal coordinates comprise a linear displacement of said one rigid body with respect to said another rigid body (p. T-10, paragraph 7, lines 1-6).

22. As per claim 8, the applicant's admitted prior art teaches said internal coordinates comprise an angular displacement of said one rigid body with respect to said another rigid body (p. T-10, paragraph 7, lines 1-6).

23. As per claim 9, the applicant's admitted prior art does not teach internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body.

However, Hollars et al teach this feature (p. R-27, paragraph 3, lines 1-6).

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art and Hollars et al. Hollars et al's teaching of internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body would have helped resolve difficulties and limitations in using other coordinate systems for bodies connected by a ball joint or a six-degree-of-freedom joint.

24. As per claim 10, the applicant's admitted prior art teaches M comprises a system mass matrix (p. 6, lines 16-17).

25. As per claim 22, the applicant's admitted prior art does not teach model comprises a plurality of rigid bodies, each rigid body representing a portion of said molecule, and a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies.

However, Hollars et al teach these features (p. T-10, paragraph 4, lines 1, 2, 3; paragraph 7, lines 1-6)

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art and Hollars et al since molecular structures are very similar to those structures described in Hollars' manual. Hollars et al's teaching of model comprises a plurality of rigid bodies, each rigid body representing a portion of said molecule, and a plurality of hinge connections, each hinge connection defining allowable relative motion between two of said rigid bodies would have helped model molecules to apply Residual Form equations effectively.

26. As per claim 23, these limitations have already been discussed in claim 4. They are, therefore, rejected for the same reasons.

27. As per claim 24, the applicant's admitted prior art does not teach internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body.

However, Hollars et al teach this feature (p. R-27, paragraph 3, lines 1-6).

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art and Hollars et al. Hollars et al's teaching of internal coordinates comprise Euler parameters of said one rigid body with respect to said another rigid body would have helped resolve difficulties and limitations in using other coordinate systems for bodies connected by a ball joint or a six-degree-of-freedom joint.

28. As per claim 25, these limitations have already been discussed in claim 6. They are, therefore, rejected for the same reasons.

29. As per claim 26, these limitations have already been discussed in claim 7. They are, therefore, rejected for the same reasons.

30. As per claim 27, these limitations have already been discussed in claim 8. They are, therefore, rejected for the same reasons.

31. As per claim 28, these limitations have already been discussed in claim 9. They are, therefore, rejected for the same reasons.

32. As per claim 29, these limitations have already been discussed in claim 10. They are, therefore, rejected for the same reasons.

Claims 11 and 30 are rejected under 35 U.S.C. 103(a) as being unpatentable over applicant's admitted prior art as applied to claim 1, 4, 5, 6, 20, 23, 21, and 24 and above, and further in view of Michael Hollars et al (SD/FAST User's Manual, Version B.2, 1994,

Symbolic Dynamic Inc,) and Eichberger et al (The Benefits of Parallel Multi-body Simulation, International Journal for Numerical Methods in Engineering, Vol. 37, pp. 1557-1572 (1994)).

33. As per claim 11, the applicant's admitted prior art and Hollars et al do not teach the f comprising a bias-free hinge torque.

However, Eichberger et al teach this feature (p. 1559, lines 12-22. These are equations in terms of generalized coordinates, speed, and time variables as described by the applicant's claimed equations).

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art, Hollars et al and Eichberger. Eichberger's teaching the f comprising a bias-free hinge torque would have simplified the motion equations and reduced time and resource to solve them.

34. As per claim 30, the applicant's admitted prior art and Hollars et al do not teach the f comprises a bias-free hinge torque.

However, Eichberger et al teach this feature (p. 1559, lines 12-22. These are equations in terms of generalized coordinates, speed, and time variables as described by the applicant's claimed equations).

It would have been obvious to one of ordinary skill in the art to combine the teachings of the applicant's admitted prior art, Hollars et al and Eichberger. Eichberger's teaching the f comprising a bias-free hinge torque would have simplified the motion equations and reduced time and resource to solve them.

Conclusion

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Cuong Luu whose telephone number is 571-272-8572. The examiner can normally be reached on Monday – Friday 8:30 AM – 5:00 PM.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Jean Homere can be reached on 571-272-3780. The fax phone number for the organization where this application or proceeding is assigned is 703-872-9306. Any inquiry of a general nature or relating to the status of this application should be directed to the TC2100 Group Receptionist: 571-272-2100.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

CVL



JEAN R. HOMERE
PRIMARY EXAMINER